Molecular Dynamics & Theoretical Chemistry

8 March 2013

Michael R. Berman

Program Officer
AFOSR/RTE
Air Force Office of Scientific Research

Integrity ★ Service ★ Excellence

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2013 AFOSR SPRING REVIEW
3002N PORTFOLIO OVERVIEW

NAME: Michael R. Berman

<u>BRIEF DESCRIPTION OF PORTFOLIO</u>:

Research on understanding and exploiting chemical reactivity and energy flow in molecules to improve Air Force systems, processes, and materials.

From a molecular perspective, understanding reaction mechanisms and developing predictive capabilities.

Understanding and utilizing chemical reactivity and catalysis for improved storage and utilization of energy

<u>LIST SUB-AREAS IN PORTFOLIO</u>:

Molecular Dynamics

Theoretical Chemistry

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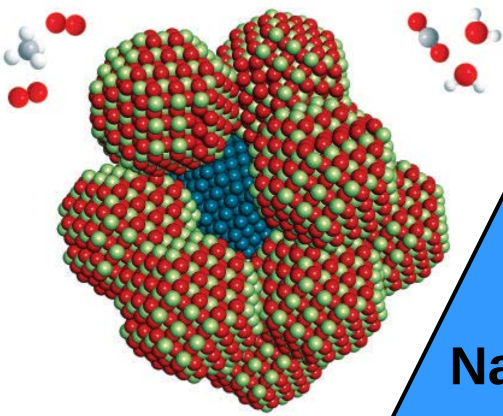
Program Synergies

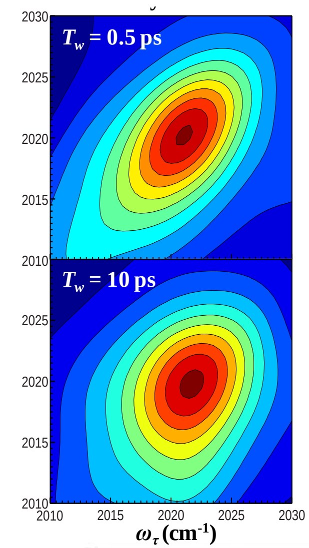


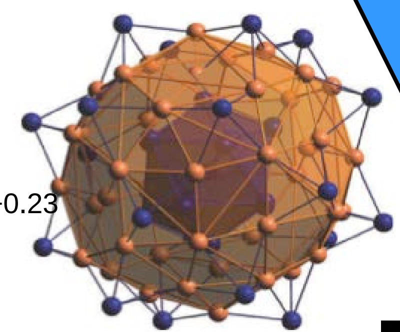
Lasers & Diagnostics

Nanostructures & Catalysis

Atm/Space/Ion Chemistry

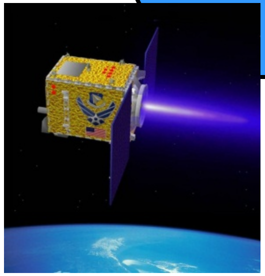
Energetic Materials





$Al^{+0.23}$

$Al_{77}[N(SiMe_3)_2]_{20}$



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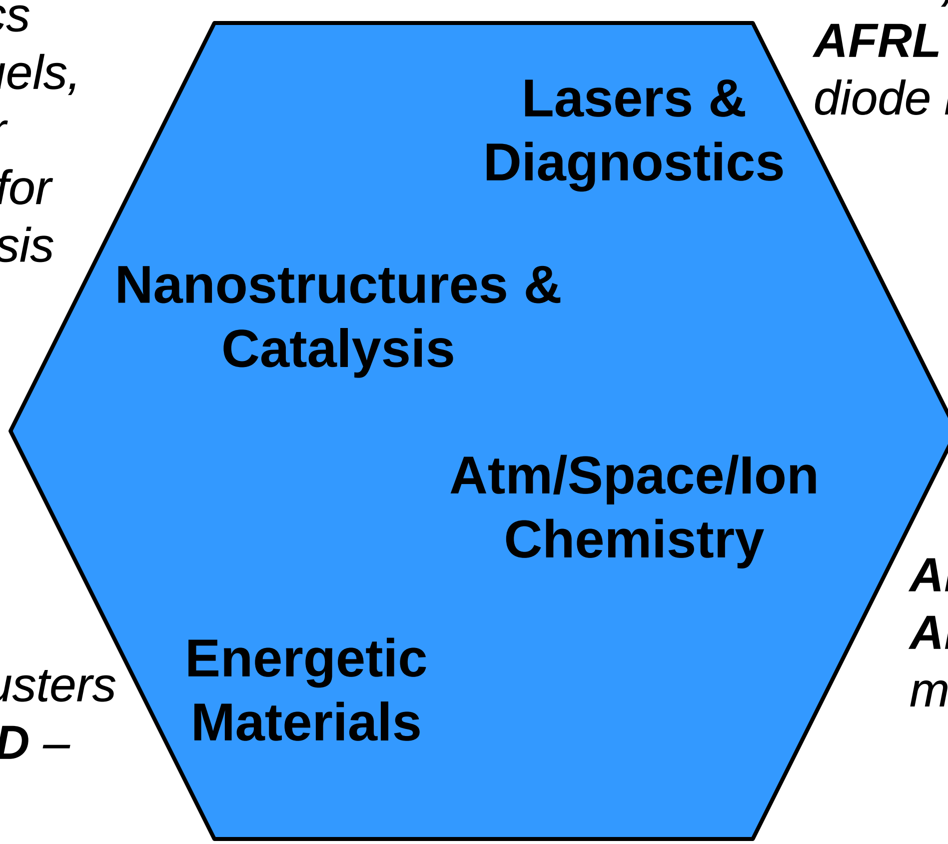
Program Interactions

AFRL, AFOSR *– XPAL, etc.*
AFRL *– ultrafast methods, diode laser spect (ICOS)*

ARO *– plasmonics*
AFOSR *- Endo fuels, combustion, solar*
PNNL *– Institute for Integrated Catalysis*



AFRL, PSI, SSI *- Codes*
AFOSR *- Simulation methods, PIs*

Navy, DTRA *– Clusters*
AFRL, NASA, DoD *– Ionic Liquids*

AFRL *– RQ, RV, RX, RW Quantum Chemistry Codes*

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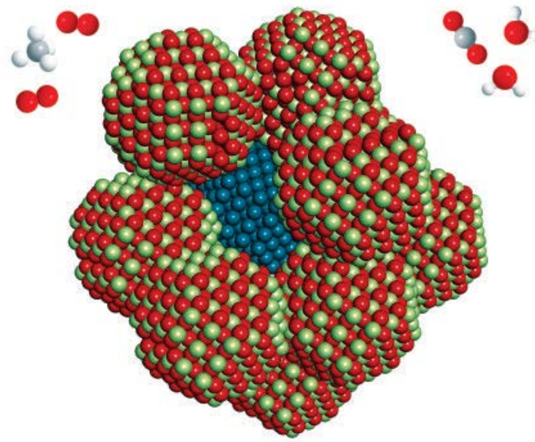
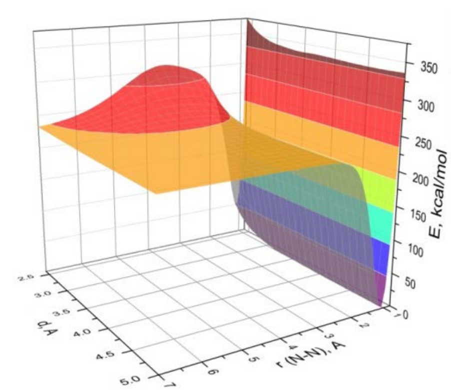
Scientific Challenges

- **Storing energy in chemical bonds as fuels/propellants/munitions**
  - $CO_2 \rightarrow$ JP8
- **Creating novel materials from nanoscale building blocks that can control energy flow**
  - Predict, prepare, probe
- **Predicting and controlling energy transfer in complex, reactive environments**
- **Probing processes at interfaces**





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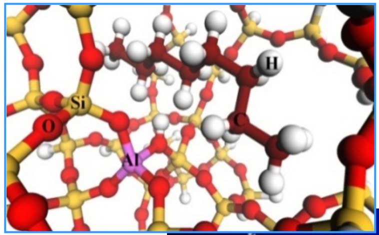
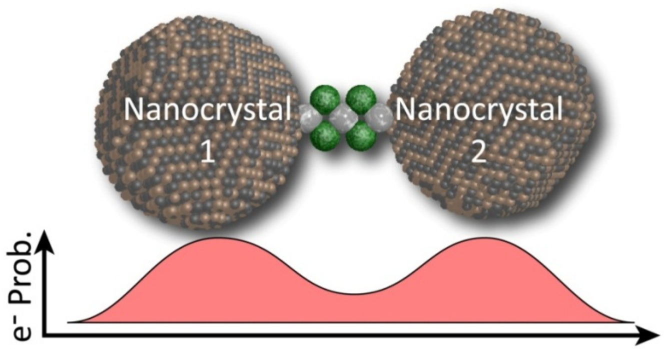
BRI Topics

- **Catalysis for Endothermic Fuels**
- **Foundations of Energy Transfer**





- **Plasma-Surface Interactions**
- **Nanoscale Building Blocks for Novel Materials**

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Program Trends

- Catalysis
- Nanostructure Assemblies
- Plasma-Surface Interactions

- Ionic Liquid Propellants
- Real-time probing of reactions

- Hybrid Chemical Lasers
- Sensors for Trace Detection

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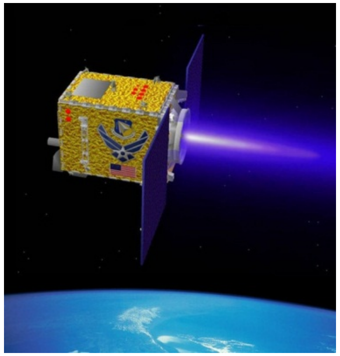
AFRL Ionic Liquid Selected by NASA as Green Propellant

- *Ionic Liquid propellant developed by AFRL (AF-M315E; Hawkins et al) with support from AFOSR selected by NASA for "Green Propellant Infusion Mission"*
- *NASA will invest $45M over 3 years*
- *Bridges gap between tech development and use*
- *Fly and characterize high performance green propellant in space in an integrated propulsion system- Falcon launch in 2015*
- *Team selected includes Ball Aerospace, Aerojet, AFRL, NASA*

AF-M315E

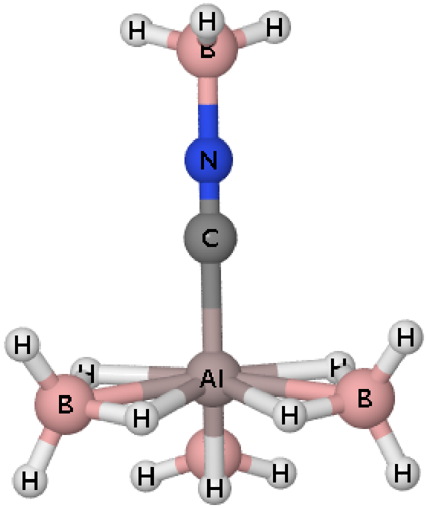
Monopropellant thruster

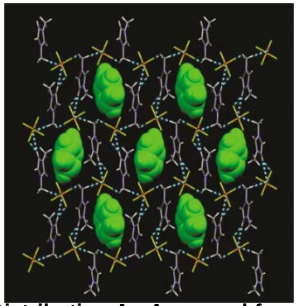


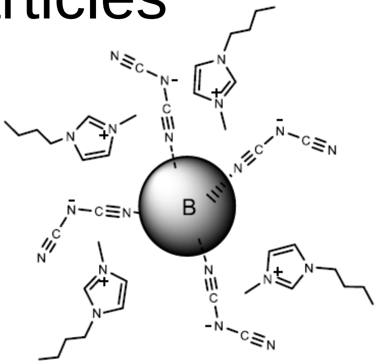
"A high performance green propellant has the potential to revolutionize how we travel to, from and in space" Michael Gazarik, Director of NASA's Space Technology Program.

New Ionic Liquids for Propellants

- Alumino-cyanoborohydride anions
  - Bipropellant fuel approach with high hydrogen content & large $\Delta H_{combustion}$
  - Hypergolic
- Additives to control energy and physical properties of ionic liquids
  - Graphenes greatly lower IL viscosity as internal 'lubricant' & increase reactivity
- Ionic liquids with metal nanoparticles
  - Passivating B and Al metal nps
- Liquid clathrates







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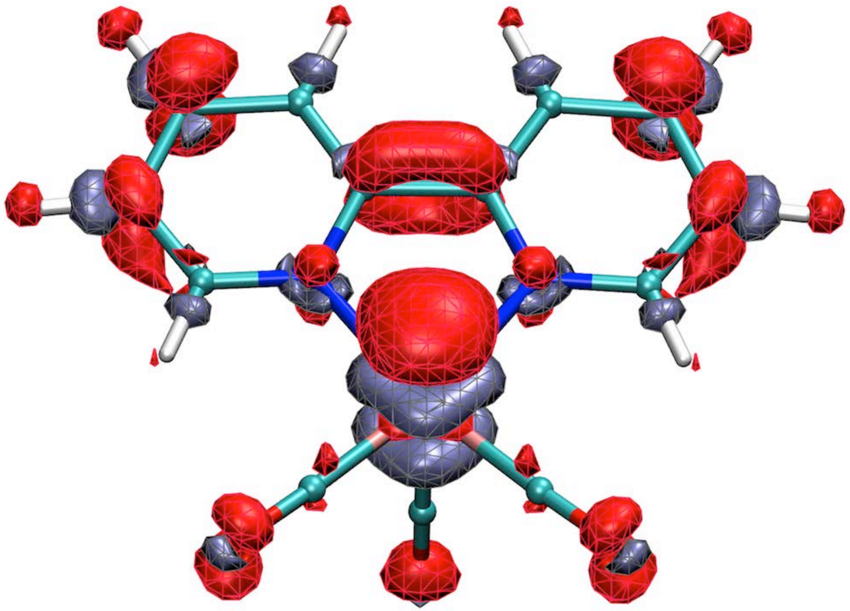
Mechanism of CO_2 Reduction

- Why is rhenium-based catalyst efficient at CO_2 reduction to CO?
  - hydride reduction is energetically favored, but CO_2 reduction dominates
- Make, model, measure approach
  - Synthesis
  - DFT studies
  - X-ray probing
- Oxidation state is $Re^0(bpy)^{-1}$. Ligands are actively involved in bonding
- HOMO permits ***σ-bonding*** and ***π-bonding;*** favors CO_2 binding
- Understanding mechanism permits ways to find alternative catalysts with similar electronic structure (Mn).



$Re(bpy)(CO)_3(L)$

Kubiak and co-workers, Angew. Chem., 2012
MURI
Kubiak, UCSD
Nilsson, Stanford
Carter, Princeton

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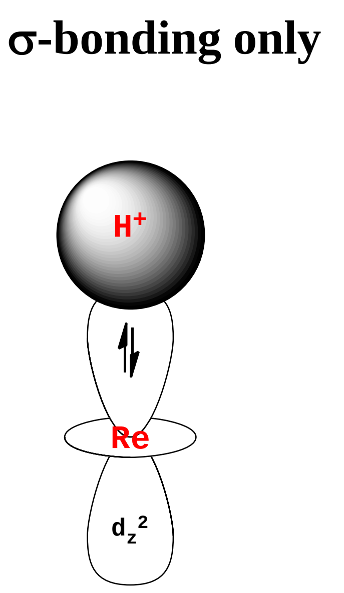
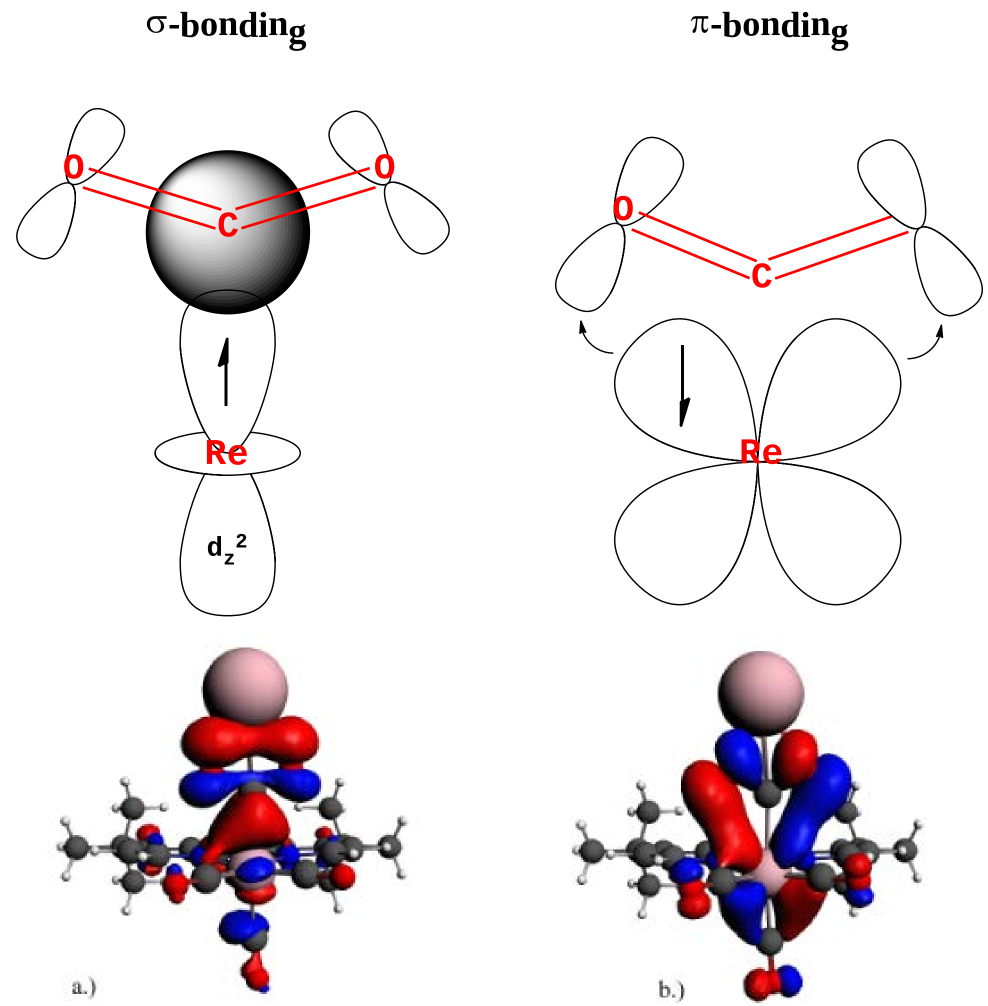
Proton Reduction vs. CO_2 Reduction





Smieja, Benson, Kumar, Grice, Seu, Miller, Mayer, Kubiak ; *PNAS* ***109,*** *15646 (2012).*

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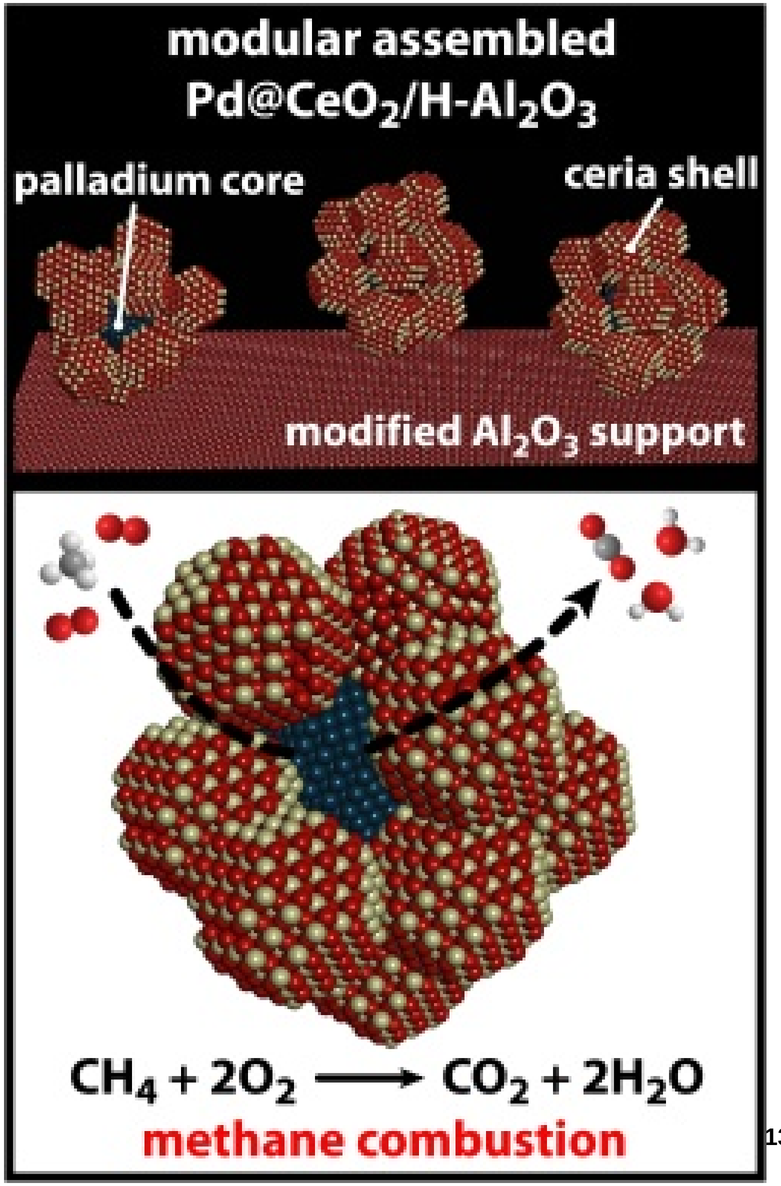
New Catalyst for Efficient, Low Temperature Methane Combustion

- Novel self-assembled core-shell nanocatalyst
  - 1.8 nm Pd core; Ceria shell
  - PdO forms at interface: active catalyst
- Complete burning of methane at 400°C
- 30 times more efficient than previous catalysts
- Applications:
  - Efficient turbines
  - Steam reforming; WGS
  - Reduce methane in exhausts

Gorte, U Penn (MURI)
Science, 337, 713 (2012)



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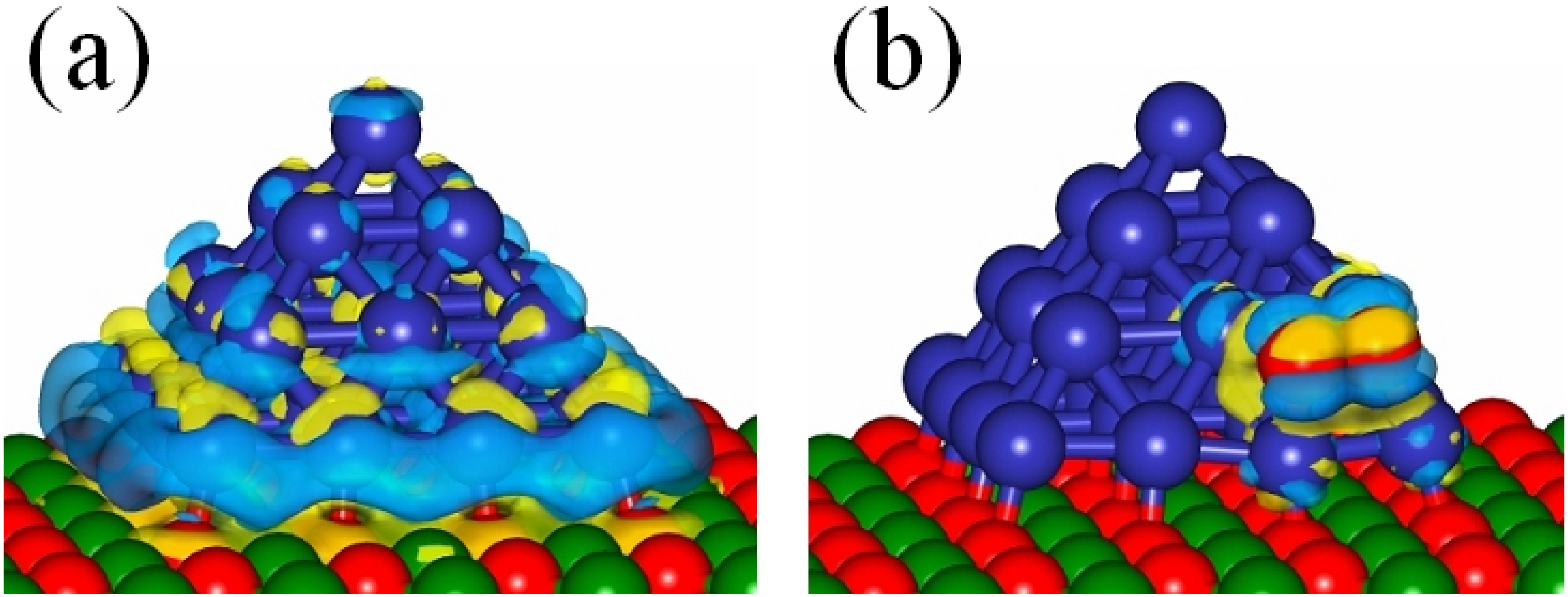
Catalysis by Pd_{30} Clusters on MgO



- Charge transfers from MgO substrate to Pd_{30} cluster at the interface
- Charge (0.25e) goes into anti-bonding orbital of adsorbed O_2
- Reaction stops when extra charge is used up (self-limiting)

Heiz (Munich); Landman (Georgia Tech)
J. Phys. Chem. C 116, 9594 (2012)

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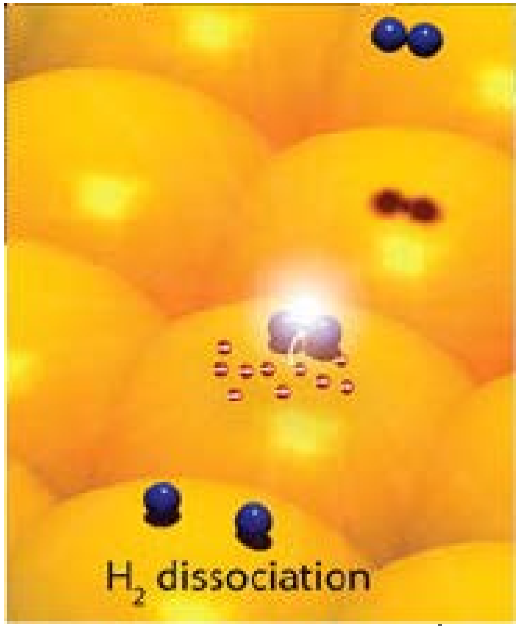
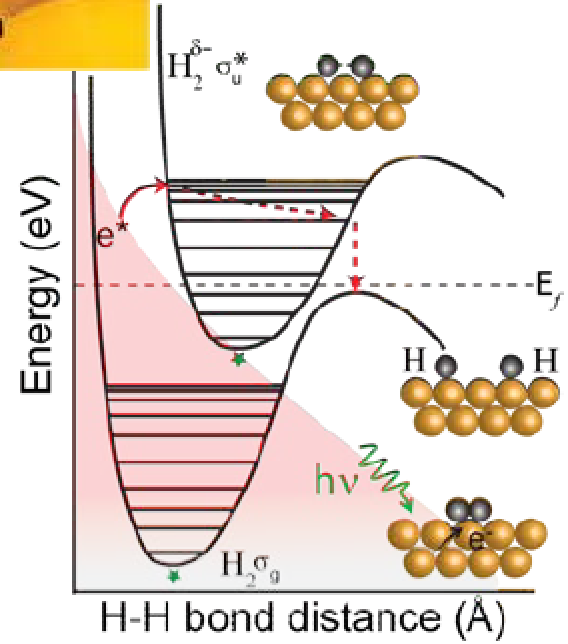
Plasmon-induced Dissociation of H_2 on Gold Nanoparticles

- Visible light excites surface plasmons in Au NP
- Plasmons decay into hot electrons (and holes) with energy below metal work function
- Hot e’s transfer to Feshbach resonance of H_2 adsorbed to Au NP triggering dissociation
- New pathway for controlling chemical reactivity on metal catalysts





Halas (Rice U); Carter (Princeton U)

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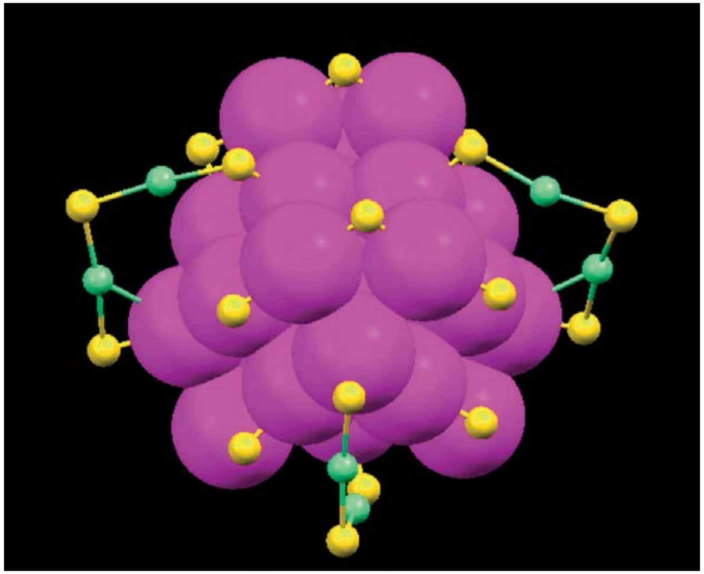
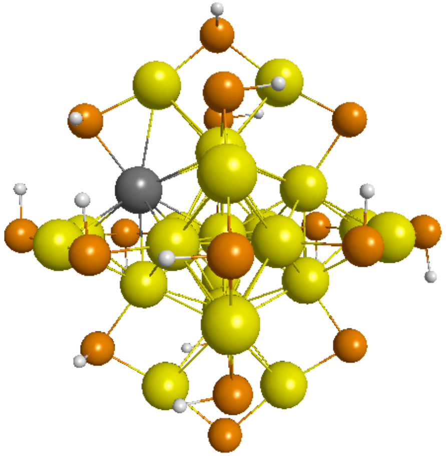
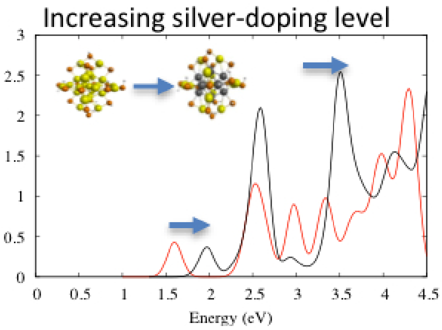
Properties of Gold Thiolate Nanoparticles

- Total Structure and Electronic Properties of the Gold Nanocrystal $Au_{36}(SR)_{24}$ determined
  - Au_{28} FCC-type tetrahedral core
  - 12 ligands bind to core as bridges
  - 12 ligands bind as “staples”
- Doping with silver atoms provides way to tune optical properties
  - Silver atoms minimize contact with other silver atoms
  - Shifts position and intensity of peaks



Jin (Carnegie Mellon); Landman (Ga Tech), Angew. Chem. Int’l. Ed. 51, 1 (2012)





Aikens (Kansas State U.) and coworkers, J. Phys. Chem. C 116, 20617 (2012)

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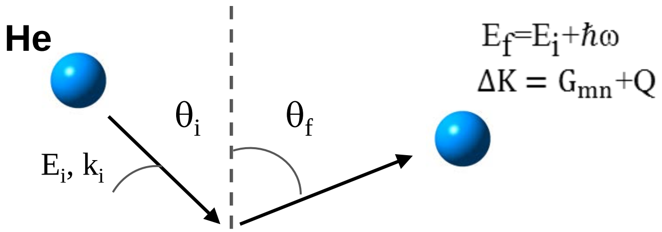
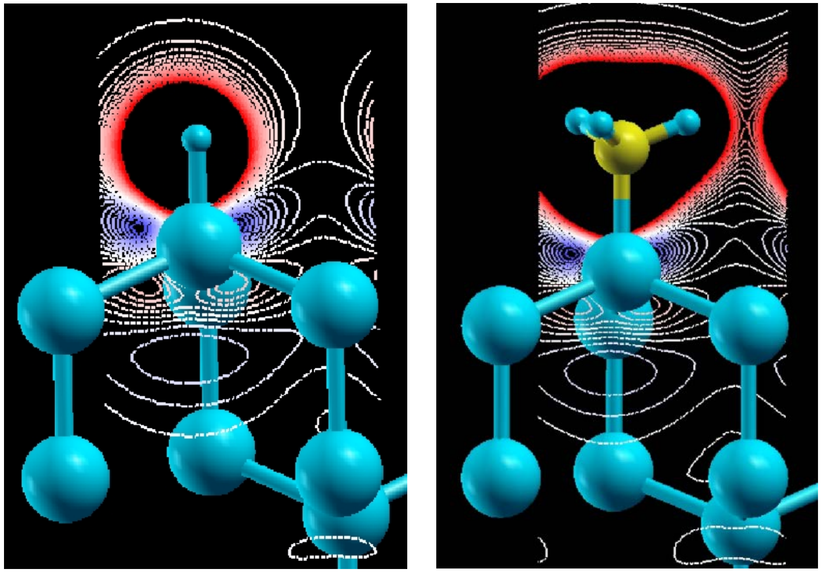
Atom Scattering to Probe Molecular Properties and Interactions

- Elastic and inelastic He atom scattering, STM, & synthesis create new electronic interfaces
- CH_3-Si(111) offers superior chemical and structural stability compared to H-Si(111)
- Air- and electrochemical-stability enables advanced sensors, fuel and solar cells, etc.
- Probes defects (electron traps) and surface librations (bonding, electron–phonon coupling)
- Provides information not attainable with IR/Raman





Sibener, (U. Chicago)
J. Chem. Phys. 133,10470 (2010);
Faraday Discussion 157, 307-323 (2012)

Synthesis: Lewis (Caltech)
Modeleing: Benedek (Milan)

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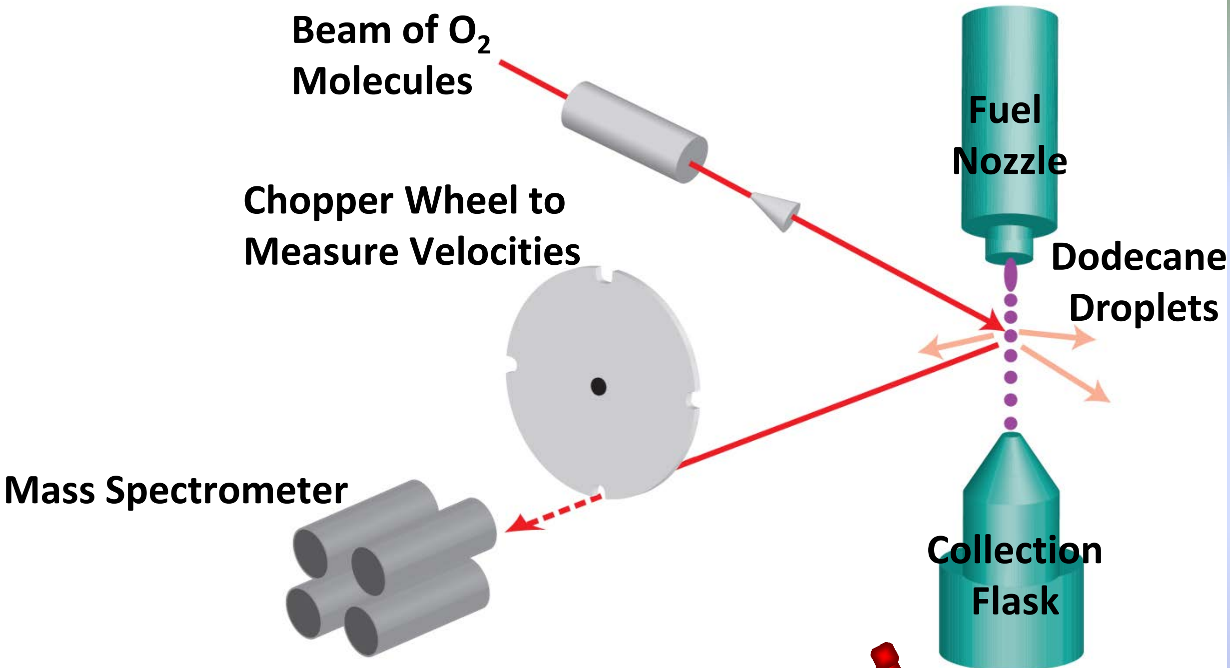
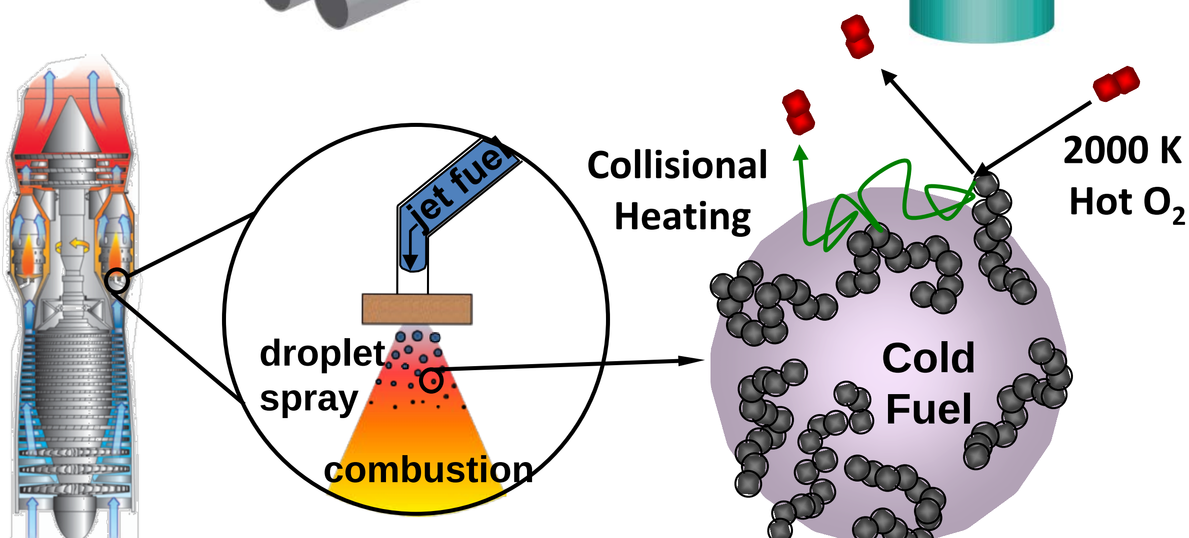
Jet Fuel Heating by Hot Gases





- Understanding fundamental processes in fuel droplets:
  - *Heating (energy transfer)*
  - *Reactions*
  - *Evaporation*
- To model this process, we direct hot O_2 molecules at liquid dodecane in vacuum
  - *Enabled by liquid microjets*
- O_2 molecules transfer ~2/3 of their energy upon collision with dodecane.
  - *Rapidly heats surface of the droplet*
  - *Fuel evaporation is not limited by gas-liquid collisions, but by heat transfer in the gas phase*.

Nathanson, U. Wisconsin-Madison

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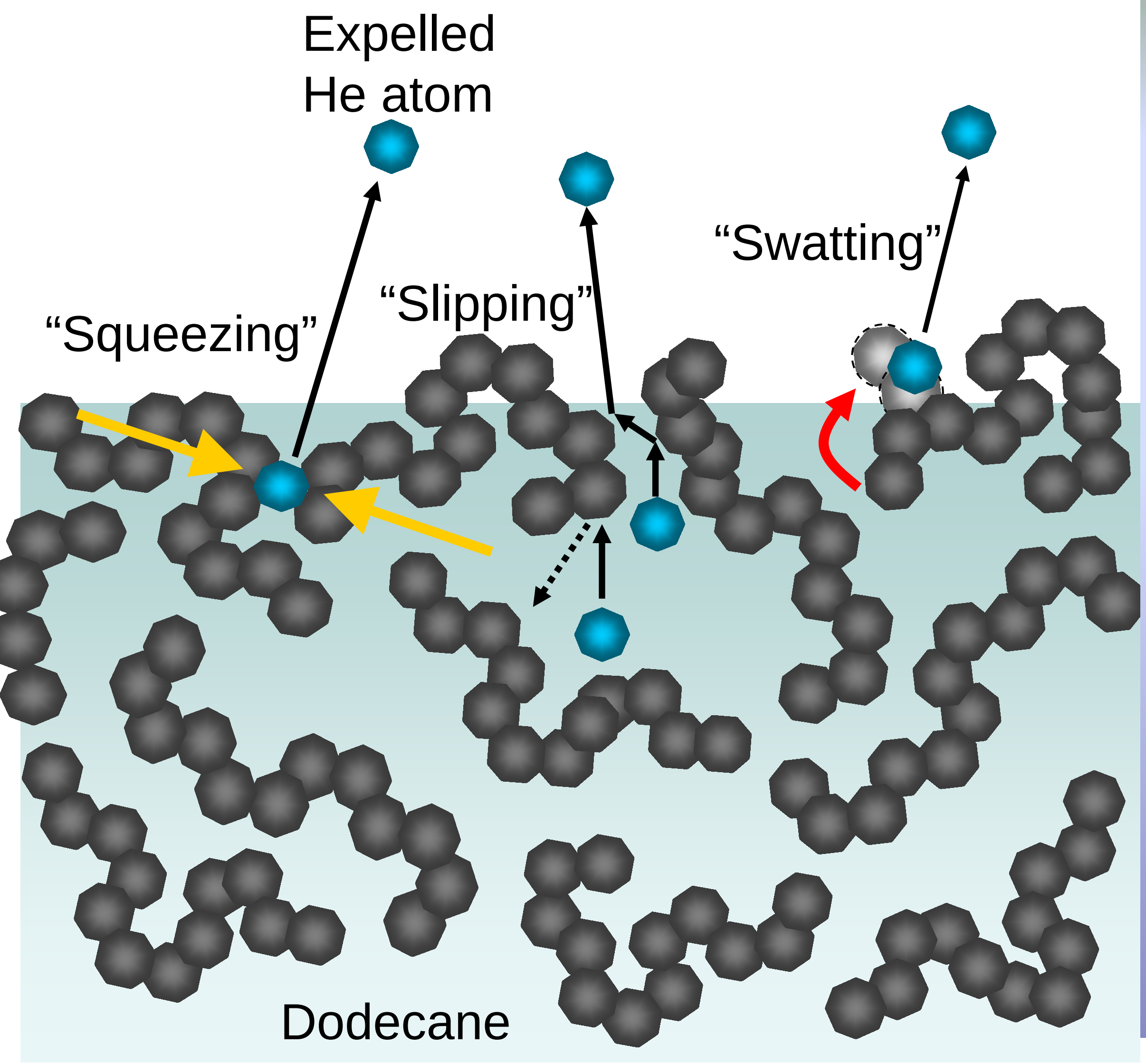
The Last Leap of a Gas Atom Off the Surface of a Liquid



- He atoms dissolved in dodecane evaporate with kinetic energies much higher than expected.
- Fast He atoms “zoom” ballistically off the surface after moving through fluctuating gaps between molecules.
  - *Squeezing*
  - *Slipping*
  - *Swatting*
- He atoms are expelled from the surface before they can thermally re-equilibrate.
- Learn how different components of jet fuel mix with each other and alter the motions of gas molecules

Nathanson, U. Wisconsin-Madison

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Feng Zhang, Li Xu, Kun Zhang, Erkang Wang, and Jin Wang

J. Chem. Phys. **137**, 065102 (2012); http://dx.doi.org/10.1063/1.4734305 (*19 pages*)

Online Publication Date: 8 August 2012

Full Text: **Read Online** (HTML) | **Download PDF**

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+ Show PACS

Merged-beams for slow molecular collision experiments

Qi Wei, Igor Lyuksyutov, and Dudley Herschbach

J. Chem. Phys. **137**, 054202 (2012); http://dx.doi.org/10.1063/1.4739315 (*9 pages*)

Online Publication Date: 6 August 2012

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Dissociative electron attachment to C_2F_5 radicals

Sean A. Haughey, Thomas A. Field, Judith Langer, Nicholas S. Shuman, Thomas M. Miller, Jeffrey F. Friedman, and A. A. Viggiano

J. Chem. Phys. **137**, 054310 (2012); http://dx.doi.org/10.1063/1.4738759 (*8 pages*)

Online Publication Date: 3 August 2012

Full Text: **Read Online** (HTML) | **Download PDF**

+ Show Abstract

Summary

- Molecular approach key to energy storage and utilization
- Clusters and nanostructures key to exploiting catalysis, plasmonics, and novel materials
- Knowledge of molecular mechanisms is key in developing and optimizing more efficient catalysts
- AFOSR leading the way in applying new tools to understand energy transfer, reaction, and catalytic mechanisms
- Many new areas of opportunity:
  - Exciton dynamics
  - Ultracold chemistry

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Challenges in Chemical Dynamics

Molecular Dynamics, Theoretical Chemistry

- **Energetic Materials** — *(Rocket propellants, explosives)*
  - Energetic ionic liquids ⇨ CHNO limit; new approaches
  - Energetic nanostructures ⇨ Sensitivity, mechanisms
  - Non-traditional concepts ⇨ Safer, penetrating munitions
- **Nanostructures/Catalysis** — *(Energy, Catalysis, Sensing)*
  - Nanostructures for catalysis ⇨ Atomic scale imaging and control
  - Photoelectrocatalysis ⇨ Activity and stability
  - Surface-plasmon enhancement ⇨ Size-dependent properties
- **Atm/Space Chemistry** — *(Signatures, surveillance)*
  - Upper atmosphere, space ⇨ Hypersonic prop, gas/surf interact.
  - Signatures & backgrounds ⇨ Rates/mech. of ion-molecule proc's.
  - Ion & plasma processes ⇨ Predictive codes, communication
- **Lasers and Diagnostics** — *(Infrared lasers, missile defense)*
  - High-Power Gas Lasers ⇨ Efficient pumping, energy transfer
  - Novel analytical tools/methods ⇨ Relaxation processes

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Interactions within AFOSR through BRIs

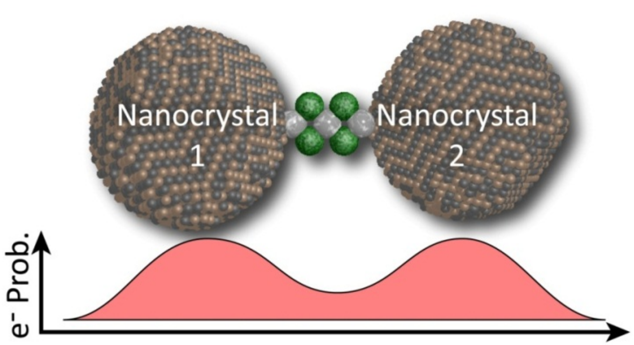
Nanoscale Building Blocks for Novel Materials
with RTD (De Long)

Use <u>nanoscale structures</u> as <u>building blocks</u> to make novel materials with new properties for energy manipulation

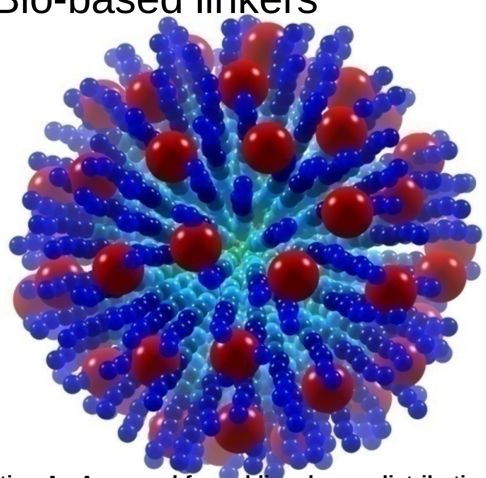
Plasma-Surface Interactions
with RTD (Luginsland)

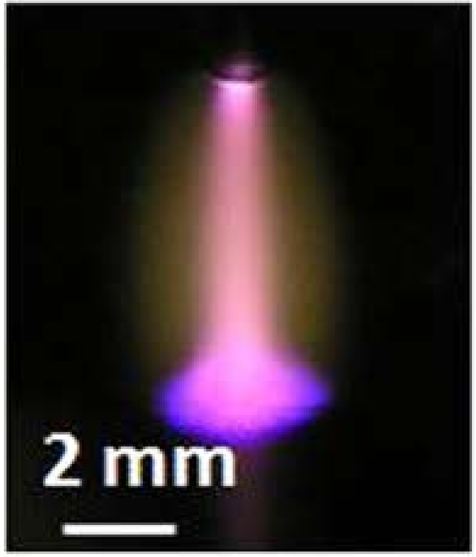
Plasma-surface interactions for enabling novel and energy-efficient means of protecting or creating materials

Chemical linkers



Bio-based linkers





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AFOSR Molecular Dynamics and Theoretical Chemistry – Active Grants 2012

Principal Investigator	Institution	Grant Title	Link
Aikens, Christine	KANSAS STATE UNIVERSITY	STRUCTURE AND OPTICAL PROPERTIES OF NOBLE METAL NANOPARTICLES	
Anderson, Scott	UNIVERSITY OF UTAH	(MURI 08) - NANOCATALYSTS IN PROPULSION: MECHANISMS AND OPTIMIZATION	
Bartlett, Rodney	UNIVERSITY OF FLORIDA	MOLECULES AND THEIR INTERACTIONS	
Bergman, Robert	UNIVERSITY OF CALIFORNIA, BERKELEY	(NII) NOVEL CATALYTIC, SYNTHESIS METHODS FOR MAIN GROUP	
Bernskoetter, Wesley	BROWN UNIVERSITY	(YIP 11) Acrylate Formation from CO2 and Ethylene by Catalysis	
Bernstein, Elliot	COLORADO STATE UNIVERSITY	STUDY OF HETEROGENEOUS CATALYTIC REACTIONS THROUGH GAS PHASE, NEUTRAL TRANSITION	
Betley, Theodore	HARVARD COLLEGE	(YIP 11) Bifunctional catalysts for CO2 reduction	
Bocarsly, Andrew	PRINCETON UNIVERSITY	PHOTOELECTROCHEMICAL CONVERSION OF CARBON DIOXIDE TO ALCOHOLS: FORMATION CARBON-BASED FUELS VIA CARBON-CARBON BOND FORMATION	
Bowen, Kit	JOHNS HOPKINS UNIVERSITY	TOWARD THE DEVELOPMENT OF ALUMINUM CLUSTER-CONTAINING MATERIALS	
Bowers, Michael	UNIVERSITY OF CALIFORNIA SANTA BARBARA	LITIGATED METAL CLUSTERS - STRUCTURES, ENERGY AND REACTIVITY	
Brown, Seth	UNIVERSITY OF NOTRE DAME	(NII) Catalytic activation of nitrogen dioxide for selective synthesis	
Carter, Emily	PRINCETON UNIVERSITY	DESIGNING NEW MATERIALS FOR CONVERTING SOLAR ENERGY TO FUELS VIA QUANTUM MECHANICS	
Castleman, A. Welford	PENNSYLVANIA STATE UNIVERSITY	CLUSTER DYNAMICS: LAYING THE FOUNDATION FOR TAILORING THE DESIGN OF CLUSTER ASSEMBLED NANOSCALE MATERIALS	
Chirik, Paul	PRINCETON UNIVERSITY	(NII) - Synthesis of Fuels and Value-Added Nitrogen-Containing	
Christe, Karl	UNIVERSITY OF SOUTHERN CA LIF	POLYNITROGEN CHEMISTRY	
Crim, Fleming	UNIVERSITY OF WISCONSIN	USING VIBRATIONS TO PROBE AND CONTROL PHOTOISOMERIZATION IN LIQUIDS	

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Cuk, Tanja	**UNIVERSITY OF CALIFORNIA BERKELEY**	**(YIP 12) In-Situ UV-VIS and IR Spectroscopy of Water OxidationCatalysts**	
Dlott, Dana	UNIVERSITY OF ILLINOIS CHAMPAIGN	ULTRAFAST DYNAMICS OF ENERGETIC MATERIALS	
Dukovic, Gordana	UNIVERSITY OF COLORADO	Photophysics and Photochemistry of Nanocrystals with Ultrashort Ligands	
Duncan, Michael	UNIVERSITY OF GEORGIA	Structure, Bonding and Surface Chemistry of Metal Oxide Nanoclusters	
Eichhorn, Bryan	UNIVERSITY OF MARYLAND	(NII) SYNTHESIS AND CHARACTERIZATION OF ALUMINUM BIMETALLIC NANOPARTICLES	
Engel, Gregory	UNIVERSITY OF CHICAGO	(PECASE) - HARNESSING SOLAR POWER NOVEL STRATEGIES FOR RATIONAL DESIGN OF PHOTOCATALYSTS AND PHOTOVOLTAIC MATERIALS	
Fayer, Michael	STANFORD UNIVERSITY	Dynamics and Interactions in Ionic Liquids and Surfaces	
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